Short Communication: The Wasserstein distance as a dissimilarity metric for comparing detrital age spectra, and other geological distributions

Accepted, peer-reviewed manuscript, compiled May 17, 2023

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Abstract

Distributional data such as detrital age populations or grain size distributions are common in the geological sciences. As analytical techniques become more sophisticated, increasingly large amounts of distributional data are being gathered. These advances require quantitative and objective methods, such as multidimensional scaling (MDS), to analyse large numbers of samples. Crucial to such methods is choosing a sensible measure of dissimilarity between samples. At present, the Kolmogorov-Smirnov (KS) statistic is the most widely used of these dissimilarity measures. However, the KS statistic has some limitations such as high sensitivity to differences between the modes of two distributions, and insensitivity to their tails. Here we propose the Wasserstein-2 distance (W_2) as an additional and alternative metric for use in geochronology. Whereas the KS-distance is defined as the maximum vertical distance between two empirical cumulative distribution functions, the W_2-distance is a function of the horizontal distances (i.e., age differences) between observations. Using a variety of synthetic and real datasets we explore scenarios where W_2 may provide greater geological insight than the KS statistic. We find that in cases where absolute time differences are not relevant (e.g., mixing of known, discrete age peaks), the KS statistic can be more intuitive. However, in scenarios where absolute age differences are important (e.g., temporally/spatially evolving sources, thermochronology, and overcoming laboratory biases) W_2 is preferable. The W_2-distance has been added to the `R` package IsoplotR, for immediate use in detrital geochronology and other applications. The W_2 distance can be generalised to multiple dimensions, which opens opportunities beyond distributional data.

***K*eywords** Distributional data · Wasserstein distance · Kolmogorov-Smirnov distance · Detrital mineral ages · MDS

1 Introduction

A distributional dataset is one where the information does not lie in individual observations, but in the *distribution* of many observations associated with one sample. Such data are common in the geological sciences, for example, detrital mineral ages or grain size distributions. Zircon U-Pb ages, in igneous and detrital samples, are one particularly widely used class of distributional data, which are used *inter alia* to constrain sediment provenance, global magmatic processes, and the evolution of plate tectonics (e.g., Condie et al. 2009; Cawood et al. 2012; Reimink et al. 2021). Grainsize distributions are another common form of geological distributional data. Analytical advances mean that increasingly large amounts of distributional data are being generated in the Earth sciences meaning that qualitative comparison of samples is becoming infeasible, and objective dissimilarity metrics between samples must be used. Some measure of dissimilarity (or more specifically, distance) is also required for many widely used statistical methods such as clustering, ANOVA, and dimension reduction. Dissimilarity metrics in geochronology at present are most commonly used for dimension reducing techniques such as multi-dimensional scaling (MDS) or principal component analysis (PCA). Such methods have become popular for analysing large numbers of detrital age spectra simultaneuously (Vermeesch 2013; Sharman et al. 2018; Vermeesch 2018a). Fitting models (e.g., sediment source partitioning) using distributional data also requires a definition of dissimilarity for comparing observed and predicted distributions (e.g., Amidon et al. 2005; De Doncker et al. 2020).

For all uses, the choice of which dissimilarity metric to use is vital as different metrics result in different numerical results and thus different geological interpretations. In general, the most appropriate metric will depend on the data being analysed and the scientific question under investigation. The Kolmogorov-Smirnov (KS) distance, calculated as the maximum vertical distance between two empirical cumulative distribution funtions (ECDFs) has emerged as a 'canonical' distance metric between mineral age distributions (Berry et al. 2001; Vermeesch 2018a). However, the KS-distance has a number of drawbacks, chiefly that as only the *maximum* vertical difference between ECDFs is important, it is insensitive to variability in the tails of distributions. A number of alternative dissimilarity measures have previously been proposed to address this issue, including established methods such as the Kuiper statistic, and ad-hoc dissimilarity measures such as the 'likeness' and 'cross-correlation' coefficients (Saylor et al. 2012; Satkoski et al. 2013). Unfortunately, these alternatives have drawbacks, including a propensity for the ad-hoc dissimilarity measures to produce unintuitive results when applied to extremely large and/or precise datasets (Vermeesch 2018a).

In this paper we present an alternative to the KS-distance that does not suffer from some of these limitations: the Wasserstein distance (also known as the Earth-mover's or Kantorovich–Rubinstein distance). To introduce the chief principle behind this measure, let us consider a simple toy example. Table 1 contains four samples (*A* through *D*), each of which contains exactly one single grain analysis:

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Table 1: **A toy, single-grain per sample dataset**

Sample	A	B	C	D
Age, Ma	1	1	2	11

As the KS distance is the vertical difference between ECDFs, it is insensitive to the absolute, 'horizontal' age differences between individual observations. Thus, the KS-distances between A and the other three samples are $KS(A,B) = 0$, $KS(A,C) = 1$ and $KS(A,D) = 1$. Counter to our expectation, the KS-distance cannot 'see' the relative age difference between sample A and samples C and D. For the toy example, the Wasserstein distance simply corresponds to the horizontal distance between the four samples. Thus, $W(A,B) = 0$, $W(A,C) = 1$, and $W(A,D) = 10$, which is a more sensible result than that achieved with the KS-distance.

In the following sections, we first introduce the Wasserstein distance in a more realistic setting, and formally define it. Next we discuss how it can be decomposed into intuitive terms that accord with how qualitatively, as geologists, we might compare distributions. We then proceed to compare the Wasserstein distance to the KS distance using a simple yet realistic synthetic example. Finally, we analyse a series of case studies, analysing real datasets using both the Wasserstein and KS distances. We thus evaluate the benefits and drawbacks of both metrics, identifying scenarios when one metric may be preferred to the other. Whilst we focus primarily on detrital age distributions, we emphasise that much of the following discussion applies equally to any form of distributional data.

2 The Wasserstein distance

The Wasserstein distance is a distance metric between two probability measures from a branch of mathematics called 'optimal transport'. Optimal transport is often intuited in terms of moving piles of sand from one location to another with no loss or gain of material (e.g., Villani 2003). The problem that optimal transport solves is finding the way to transport the sand such that the least sand is moved the least distance. The Wasserstein distance is the cost associated with this most efficient transportation. The association with moving piles of sand is why the Wasserstein distance is often termed the Earth-mover's distance. Figure 1a shows an example of how one univariate probability distribution, μ, based on a detrital age spectrum, is transformed into another, ν according to the optimal transport plan. Elsewhere in the Earth sciences, the Wasserstein distance is increasingly used for solving non-linear geophysical inverse problems (e.g., Engquist and Froese 2014; Métivier et al. 2016; Sambridge et al. 2022) and has been proposed as a tool for fitting hydrographs (Magyar and Sambridge 2023). Full mathematical treatments of the Wasserstein distance and optimal transport are beyond the scope of this paper, but interested readers are referred to Villani 2003 or Peyré and Cuturi 2019. A geophysical perspective is given in Sambridge et al. 2022.

2.1 Formal definition

We consider two univariate probability distributions μ and ν which have cumulative distribution functions (CDFs) M and N respectively. The p^{th} Wasserstein distance between μ and ν is

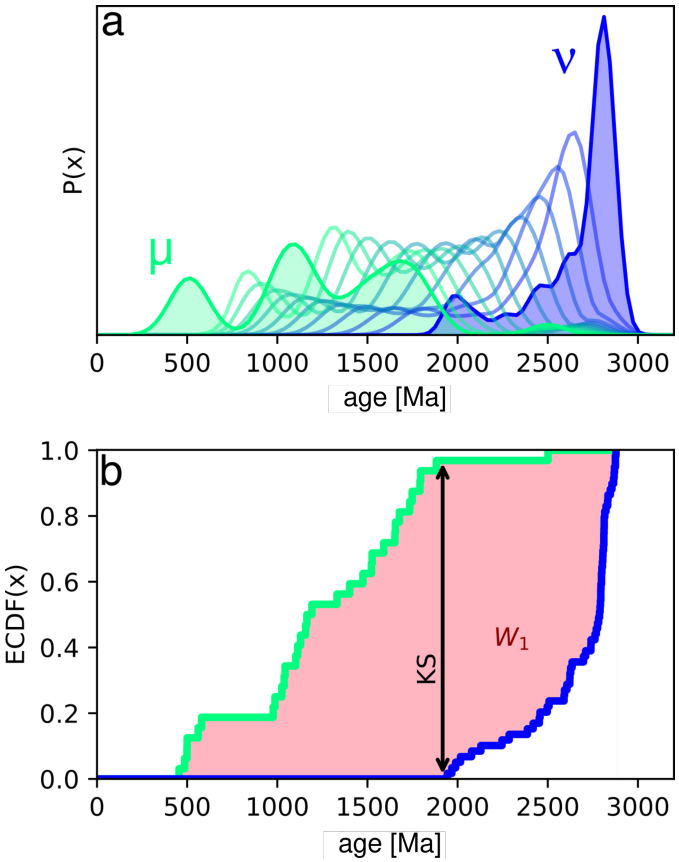

Figure 1: **Intuition of the Wasserstein distance.** a) Green and blue filled polygons show two example kernel density estimates of mineral ages from two samples (based on data from Morton et al. 2008) The distributions are labelled μ and ν for consistency with Equation 1. Semi-transparent coloured lines are probability distributions spaced equally in Wasserstein space between μ and ν (termed 'barycentres'; Benamou et al. 2015). b) Empirical Cumulative Distribution Functions (ECDFs) of the detrital ages used to calculate the distributions shown in panel a, same colours. The first Wasserstein (W_1) distance corresponds to the total area between the two ECDFs (shaded pink). The Kolmogorov-Smirnov (KS) distance is the maximum distance between the two ECDFs (black double-headed arrow).

given by:

$$W_p(\mu,\nu) = \left(\int_0^1 |M^{-1} - N^{-1}|^p \mathrm{d}t \right)^{1/p}. \tag{1}$$

where M^{-1} indicates the inverse of the CDF M and $0 \leq t \leq 1$ (Villani 2003). Note that this definition of W_p assumes that the cost-function is given by $|x-y|^p$ (e.g., the Euclidean distance where $p = 2$), which is the case for most distributional data in geology. In the further special case of $p = 1$ (i.e., the *first* Wasserstein distance, W_1), Equation 1 can be re-written simply as:

$$W_1(\mu,\nu) = \int_X |M - N| \mathrm{d}x, \tag{2}$$

which is the area between two CDFs (e.g., Figure 1b). Recall that the KS-distance between two distributions is the maximum distance between the two corresponding CDFs. Whilst the W_1

is easily visualised, we actually use the W_2 going forwards as the *squared* distance (i.e., $p = 2$) between observations is the standard distance metric in most statistical analyses (e.g., least squares regression). Additionally, W_2 decomposes into readily interpretable terms, as discussed below.

We focus on these univariate instances as they apply to the most common geological distributional data including detrital age distributions and grain size distributions. However, we note that the Wasserstein distance is, in general, multivariate. As a result, some form of the Wasserstein distance could prove useful for analysing a number of other geological datasets such as the geochemical compositions of detrital minerals, or joint U-Pb and Lu-Hf isotope analysis (see Vermeesch et al. 2023). Statistics for comparing distributional data in multiple dimensions are increasingly needed (Sundell and Saylor 2021).

Like the KS distance, W_2 satisfies the triangle inequality, and as such is a true metric. This property means that classical, as well as metric & non-metric MDS can be used with a W_2 defined dissimilarity matrix. As W_2 is sensitive to absolute time differences, metric (or classical) MDS, which seek to preserve absolute distances, may be preferable to non-metric MDS. For the rest of this manuscript, metric MDS is used.

2.2 *Decomposition*

A particularly useful property of W_2 between two univariate distributions is that it can be decomposed in terms of the differences between the two distributions' location, spread and shape. Irpino and Romano 2007 show that:

$$W_2^2(\mu,\nu) = \overbrace{(\bar{\mu}-\bar{\nu})^2}^{Location} + \overbrace{(\sigma_\mu-\sigma_\nu)^2}^{Spread} + \overbrace{2\sigma_\mu\sigma_\nu(1-\rho^{\mu\nu})}^{Shape}, \quad (3)$$

where $\bar{\mu}$ is the mean of μ, σ_μ is the standard deviation of μ and $\rho^{\mu\nu}$ is the Pearson correlation coefficient between the quantiles of the distributions μ and ν. These three terms also accord with, qualitatively, how as geologists we might compare two distributions.

2.3 *Discrete data*

Most distributional data in the Earth sciences do not, in raw form, follow continuous probability distributions. Instead, samples may be discrete sets of observations, e.g., lists of individual mineral ages. The above formulations can be easily applied to such cases by describing the probability functions μ and ν as weighted sums of δ functions. For example, let us consider two samples x_m and x_n with p and q numbers of observations respectively:

$$\mu = \sum_i^p m_i \delta_{x_m}, \quad \nu = \sum_i^q n_i \delta_{x_n} \quad (4)$$

where m and n are weight vectors, such that $\sum m_i = \sum n_i = 1$. In most geological cases these weights would be uniform, $m_i = 1/p$; $n_i = 1/q$, giving each observation within a sample equal weight. In this scenario, M and N are the familiar empirical cumulative distribution functions (ECDF), given as a series of step functions (e.g., Figure 1b).

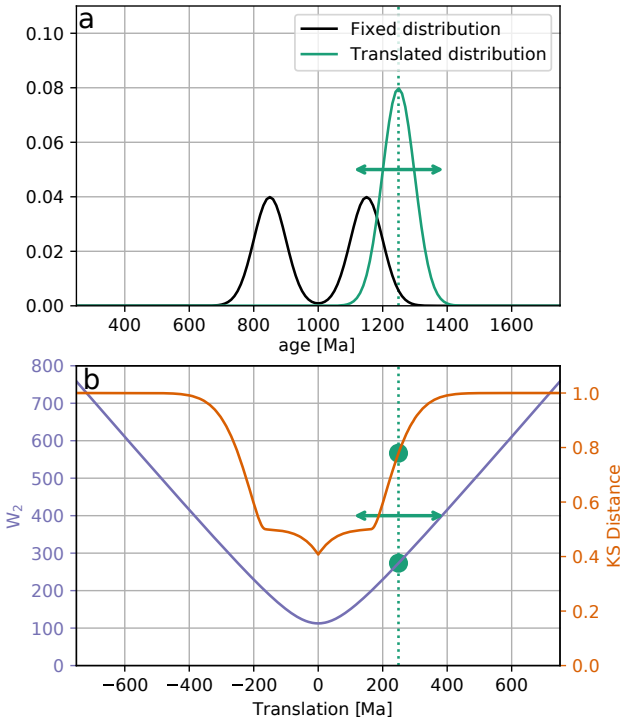

Figure 2: **Comparing the Wasserstein distance to the Kolmogorov-Smirnov distance.** a) Two synthetic probability density functions, modelled on U-Pb age spectra. The black bimodal distribution is fixed at 1000 Ma, and the green unimodal distribution is translated along the time axis. b) For each translated distribution, we calculate the KS-distance (red line) and W_2 (blue line). The green dashed line and circles indicate values associated with the location of the green distribution shown in panel a.

2.4 *A synthetic example*

To demonstrate the intuition of W_2 we explore a simple synthetic example. We consider two probability density functions of mineral ages: a bimodal distribution and a unimodal distribution, both constructed from Gaussians with the same scale (Figure 2a). We fix the bimodal distribution at 1000 Ma, but translate the unimodal distribution along the time axis. For each translated distribution we calculate both the KS-distance and W_2. Figure 2b displays the behaviour of both distances under this scenario. The KS-distance shows an unexpectedly complex response containing a series of steps, as the peaks of the distributions align and misalign. At around ±400 Ma, once the distributions stop overlapping, the KS-distance plateaus at its maximum value of 1. By contrast, W_2 increases monotonically with increasing distance. Away from the origin, W_2 approximates a linear function of the amount of translation, as is predicted from Equation 3. At the origin, the non-zero value of W_2 is the cost of turning the unimodal distribution into the bimodal distribution without translation.

We argue that the behaviour of W_2 is more geologically intuitive than the KS-distance under this scenario. It is useful geological information if two distributions differ in their means by 400, 500 or 1000 Ma, but if the distributions do not overlap, the KS-distance is insensitive to this. The Wasserstein distance

is, by contrast, sensitive to the absolute offset between non-overlapping distributions. Additionally, the stepped response of the KS-distance under translation is undesirable. Under the simple operation of translating a unimodal distribution, we would expect our dissimilarity to increase at a constant, or at least predictable (e.g., quadratic) rate. The change of the KS-distance with translation is, unintuitively, non-linear. By contrast, the W_2 increases linearly with respect to translation.

We reiterate that at a translation of 0 Ma, W_2 (and the KS distance) is still non-zero, reflecting the fact that even when the average ages are aligned, the shapes of the uni-modal and bi-modal distributions do not match. This illustrates the tendency of W_2 in geochronological data to prioritise aligning the average ages of distributions *before* considering matching individual peaks. Such behaviour contrasts with approaches that seek to only match probability peaks neglecting any information of absolute ages (e.g., Saylor and Sundell 2016).

3 Discussion

As stated above, the most appropriate dissimilarity metric to use will depend on the scientific question being answered. In general, the Wasserstein distance is most appropriate when absolute differences along the time axis (or more generally, the x-axis) provide useful information to solving the geologic problem. The KS distance however is more appropriate when the size of the time differences between peaks is not relevant. Both the KS distance and the W_2 are calculated in terms of differences between ECDFs. Due to these similarities in construction, in many cases the results from using the KS and W_2 are, encouragingly, similar. One exception is whether ages are log transformed prior to analysis. Because the KS distance considers only the order of the ages, it will be the same whether a log transform is used or not. W_2 however will be different, and will consider *relative* not absolute age differences. Such an example is discussed below (Figure 5).

Here we discuss a variety of realistic scenarios where the KS and W_2 may result in different interpretations. In each, we evaluate the advantages and disadvantages of using W_2 or KS. These case-studies can be used to determine which metric is most appropriate for a particular scenario.

3.1 Discriminating contributions from discrete endmembers

We first consider a scenario where the samples are assumed to be mixtures, in differing proportions, of some known or unknown fixed endmembers. This situation is one where absolute distance along the time-axis is not relevant, as the nature of the endmembers is not sought, simply their relative contributions to a set of mixtures. Instead, it is *vertical* differences in the probability at a given age that is relevant. The KS distance, which is sensitive to such vertical differences in age distributions is better suited for this than W_2. Indeed, in such a scenario the W_2 can result in some unintuitive behaviour.

For example, let us consider three unimodal potential sediment sources, as shown in Figure 3a. We now consider two mixture samples. The first is an equal mixture of X and Y, and the second an equal mixture of Y and Z (bottom two plots, Figure 3a). Geologically, we would expect these samples to be about half

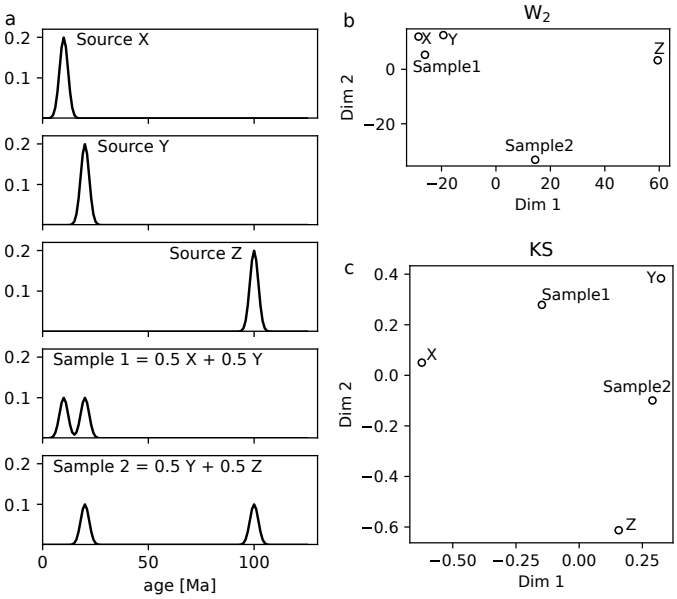

Figure 3: **Mixing of discrete endmembers** a) Three theoretical, unimodal source age distributions with peaks at 10, 20 and 100 Ma, and two mixture samples. Sample 1 is an equal mixture of X and Y and Sample 2 a mixture of Y and Z. b) Metric MDS map of the three sources and the mixtures using W_2 distance (stress = 0.05). c) Same as panel b for KS distance (stress = 0.05). This is a scenario where KS distance may be preferable to W_2.

as similar to the two source endmembers. However, a W_2 MDS map identifies these samples as being removed from their two endmembers (Figure 3b). Additionally, because of the absolute time difference between Source Z and the other sources, Sample 2 is treated as a considerable outlier. The KS distance performs better here, placing the mixtures approximately halfway between the expected endmembers. However, in such a well defined mixing scenario as this, methods such as endmember mixture modelling may be more appropriate than statistical dimension reduction (e.g., Weltje 1997; Sharman and Johnstone 2017; Dietze and Dietze 2019).

3.2 Temporally varying source age distributions

In contrast, scenarios where the shape of sediment source age distributions evolves in space and time are well suited to using W_2. This is because W_2 considers all parts of a distribution, whereas the KS only compares one point, the location of maximum ECDF separation. For example, Figure 4 displays detrital zircon age distributions gathered by DeGraaff-Surpless et al. (2002) from sediments from a section (Cache Creek) across the Great Valley Group in California, USA. The age populations are shown as KDEs and histograms, in stratigraphic order, in Figure 4a. The uppermost samples show an increasingly broad distribution than the lower four unimodal samples. DeGraaff-Surpless et al. (2002) attribute this trend, *inter alia*, to expanding sediment source areas.

Figures 4b–c display MDS maps calculated using W_2 and KS respectively. The W_2 map clearly identifies the stratigraphic order of the samples by the changing distribution shape. Additionally,

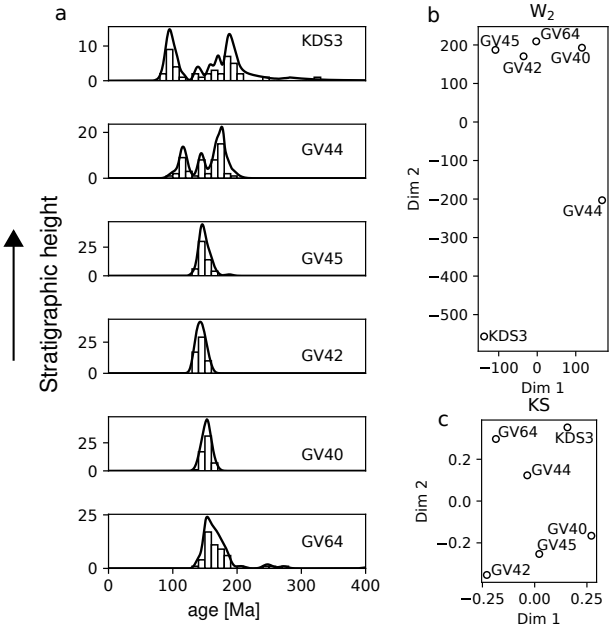

Figure 4: **Temporally evolving source distributions.** a) KDEs and histograms for zircon age distributions for samples from Cache Creek section across Great Valley Group, arranged in stratigraphic order (DeGraaff-Surpless et al. 2002). b) MDS map using W_2 for data shown in panel a (Stress = 0.28). c) Same as b using KS distance (Stress = 0.18). In this scenario, the results from W_2 are preferable.

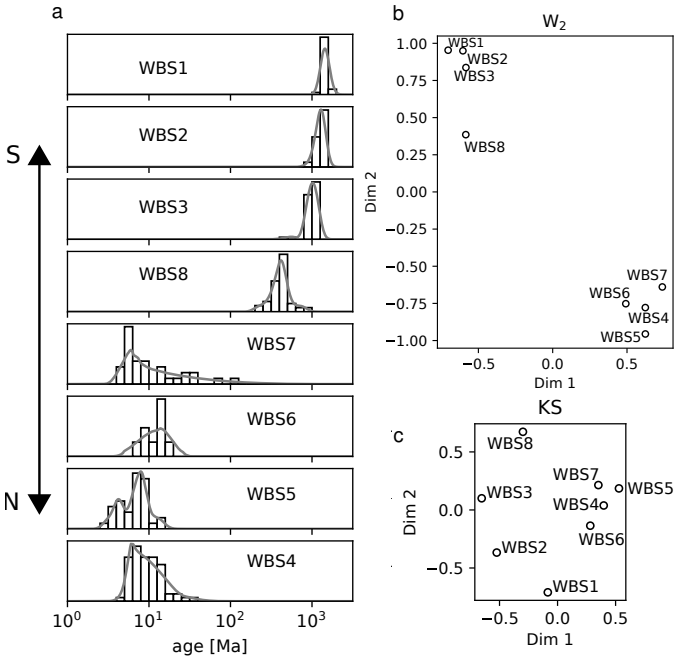

Figure 5: **Analysing thermochronological data using W_2 and KS distances.** a) KDEs for a detrital mica $^{40}Ar/^{39}Ar$ dataset of Wobus et al. (2003) arranged from south to north across a physiographic transition of the central Himalaya in Nepal. Note the logarithmic scale. b) The MDS configuration using W_2, following a log transform (stress = 0.02). c) MDS map using KS statistic (stress = 0.18). In this example, W_2 performs better than the KS distance at identifying the geographic trend.

it clusters the four unimodal samples together. By contrast, the KS map does not identify the stratigraphic trend, locating the lowermost stratigraphic sample GV64 with the uppermost samples KDS3 and GV44. We conclude then that the W_2 has better captured the geological information in this scenario.

3.3 *Thermochronology*

In thermochronology, age distributions shift along the time-axis according to thermal signals (e.g., exhumation). In many thermochronological studies, we may seek to characterise how such a signal evolves in space and time. For this question absolute distance along the time-axis is useful information and so the W_2 may be more effective than the KS distance. For example, Wobus et al. (2003) use $^{40}Ar/^{39}Ar$ detrital mica thermochronometry to explore spatially varying exhumation along a spatial transect in the Himalaya. The KDEs of the samples are shown in Figure 5a arranged south to north. The southern samples (WBS1, WBS2, WBS3, WBS8) show old exhumation signals, but a dramatic shift to younger ages is observed north of a distinct physiographic transition. MDS maps of these samples are shown using the KS distance and W_2 in Figures 5b–c respectively. As there is limited overlap between the samples, the KS distance struggles to capture the NS progression in exhumation age. Whilst the physiographic division is found, it weights it equally to variation within one cluster. By contrast, the W_2 map correctly identifies the simple temporal and geographical trend of the samples from south to north.

3.4 *Combining data from multiple laboratories*

A final scenario where the W_2 could be preferable is when comparing samples from different laboratories which are affected by inter-laboratory bias. Košler et al. (2013) provided ten different laboratories with identical synthetic zircon samples with a known age distribution. Different instruments introduced small differences in the ages of each peak. For example, in Figure 6 we display the results from Lab 1 (red) and Lab 4 (pink) as KDEs. The expected peak at ~ 1200 Ma (dashed line) is offset between the two samples. As it is the maximum distance between two ECDFs, the KS distance is very sensitive to minor offsets in sharply defined peaks. In this case, the KS distance between these theoretically identical samples is large at 0.348, which is over one third of the maximum possible distance between samples. Indeed, the KS distance considers a synthetic, purposefully misaligned series of peaks (black KDE) to be more similar to the Lab 4 results than the results from Lab 1. The W_2 distance, does not suffer from this oversensitivity to minorly offset peaks and correctly identifies the samples from Lab 1 and Lab 4 as being much more similar than the random synthetic distribution.

4 IMPLEMENTATION

We provide example code (github.com/AlexLipp/detrital-wasserstein) in both Python and R that demonstrates how to calculate the W_2 between two univariate distributions (U-Pb zircon ages). For these examples we make

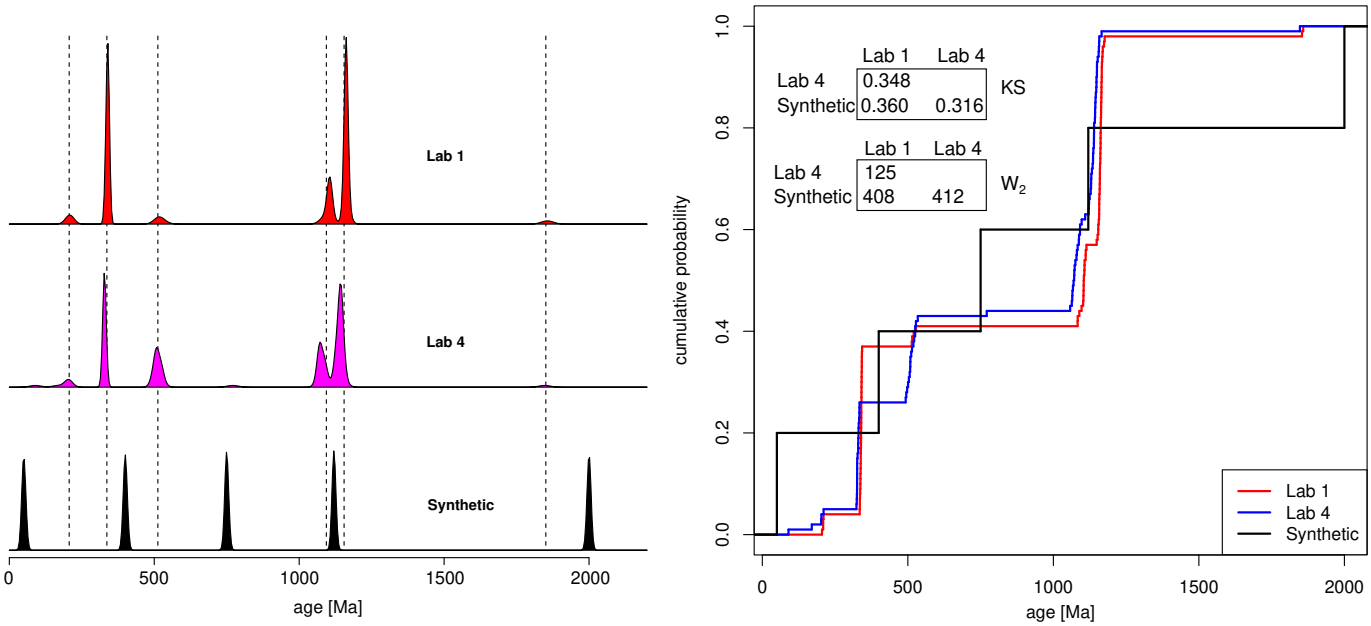

Figure 6: **Comparing samples from an inter-laboratory calibration study**. KDEs (left) and ECDFs (right) of two samples from the inter-laboratory comparison study of (Košler et al. 2013), plus a purposefully misaligned synthetic sample. Dashed lines mark the true ages of the detrital mixture. According to the KS-statistic, the age distribution produced by Lab 4 is more similar to the synthetic distribution than it is to the distribution produced by Lab 1, despite the absence of any shared age components. The W_2 distance correctly deems the distribution produced by Lab 4 to be closer to that of Lab 1 than to the synthetic mixture.

use of the the POT and transport packages in Python and R respectively which implement solutions to Equation 1 (Flamary et al. 2021; Schuhmacher et al. 2022).

4.1 IsoplotR

Additionally, the W_2-distance has been added to the IsoplotR package in R, which calculates dissimilarity matrices and MDS maps (Vermeesch 2018b). This software can be accessed using an (online) graphical user interface, at `isoplotr.es.ucl.ac.uk`. Alternatively, the function can also be accessed from the R command line. The following snippet uses W_2 to calculate an MDS map for the dataset from Wobus et al. (2003) discussed in the manuscript (Figure 5). The data required is also available at the above repository. Note that the MDS map produced may show slight differences to those in the manuscript due to dependence of metric MDS on a random state variable. This variability can introduce reflections/rotations of the data, but the underlying structure is unchanged.

```
# load the package & data
library(IsoplotR)
DZ <- read.data("wobus.csv",method="detritals")
# example 1. calculate the W2 distance matrix:
d <- diss(DZ,method="W2")
# example 2. apply MDS to the dataset:
mds(DZ,method="W2")
```

5 CONCLUSIONS

The second Wasserstein distance, W_2, is an effective metric for comparing distributional data in the geological sciences such as detrital age spectra or grain size. Unlike the KS distance, W_2 can be extended to further dimensions. W_2 is a function of the horizontal distances between observations, in contrast to the KS distance, which corresponds to vertical differences between ECDFs. Using a variety of case studies we explore scenarios where the W_2 may or may not be preferable to the KS distance. In scenarios where discrete, known age peaks are mixed, the KS distance may be preferable. However, in other scenarios where absolute differences along the time axis are useful information, W_2 is preferable. Example scenarios include spatially/temporally evolving source distributions, thermochronological data, and combining detrital samples from different laboratories. The Wasserstein distance has been added to the IsoplotR software, and example scripts are provided in Python and R.

ACKNOWLEDGEMENTS

AGL is funded by a Junior Research Fellowship from Merton College, Oxford. PV is supported by NERC Standard Grant #NE/T001518/1. This work benefited from discussions with Malcolm Sambridge & Kerry Gallagher. We thank reviews from Joel Saylor, an anonymous reviewer, and the associate editor Michael Dietze for their constructive feedback.

CODE AVAILABILITY

The code and data repository is found at `github.com/AlexLipp/detrital-wasserstein`

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